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Parallel Linear Algebra Methods

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This contribution presents two examples for the numerical treatment of partial differential equations using parallel algorithms / computers. The first example solves the Poisson equation in two dimensions; the second partial differential equation describes the physical process of vibration of a membrane. Both problems are tackled with different strategies: The Poisson equation is solved by means of the simple Jacobi algorithm and a suitable parallelization scheme is discussed; in the second case the parallel calculation is performed with the help of the ScaLAPACK library and the issue of data distribution is addressed.

1 Introduction

Numerical linear algebra is an active field of research which provided over the years many methods / algorithms for the treatment of standard problems like the solution of systems of linear equations, the factorization of matrices, the calculation of eigenvalues / eigenvectors etc.¹. The most suitable algorithm for a given linear algebra problem, e.g. arising in a scientific application, has to be determined depending on the properties of the system / matrix (see for instance Ref. 2) like:

- **symmetry**
- **definiteness** (positive, negative, . . .)
- **non-zero structure** (dense, sparse, banded)
- **real or complex** coefficients

and so on. Furthermore the scientist has to decide whether to use a **direct** solver, leading to a transformation of the original matrix and thus (for large problems) generating a need for huge **main memory**, or to use an **iterative** solver which works with the original matrix.

The same rationale holds for the more specialized field of **parallel linear algebra** methods. There the additional aspects originating from the parallel **computer architecture** have to be taken into account in order to choose a suitable algorithm. Several topics influencing the choice and even more the consequent implementation of these algorithms are^{3,4}:

- memory architecture (**shared-memory** vs. **distributed memory**)
- amount of **memory per process/processor**
- implemented **cache** structures

It is far beyond the scope of this contribution to give an overview of the available algorithms. Instead we refer to review articles like Refs. 5–7.

From a practical point of view another important decision is whether the user implements the linear algebra algorithm **himself** or relies on **available software / libraries**. A variety of well-known, robust packages providing high computational performance are on the market, which can be used as building blocks for an application software. Some **freely-available** libraries are:

- Basic Linear Algebra Subprograms (**BLAS**)⁸
- Linear Algebra Package (**LAPACK**)⁹
- Scalable LAPACK (**ScaLAPACK**)¹⁰
- (**P**)**ARPACK** - a (parallel) package for the solution of large eigenvalue problems¹¹
- Portable, Extensible Toolkit for Scientific computation (**PETSc**)¹²

Some of them like BLAS or LAPACK are **serial** software, which help to gain good single processor performance, but leave the task of **parallelization** of the high-level linear algebra computations, e.g. solution of the coupled linear equations, to the user; others, e.g. ScaLAPACK or PARPACK, contain implementations of **parallel solvers**. Thus these packages relieve the user of the parallelization, but still they rely on special data distribution schemes¹³ which require a specific organization of the application program. As a consequence the user has to handle the corresponding data distribution on his own, i.e. he has to parallelize his program at least partly. Nevertheless this might be a lot easier than to implement the full parallel linear algebra algorithm.

Since both strategies are preferable under certain circumstances, we will present in the following two simple physical problems where the **parallel numerical solution** will be demonstrated paradigmatically along the two different approaches:

In Section 2 the Poisson equation will be treated using a **parallel Jacobi solver** for the evolving system of linear equations.

In Section 3 the eigenvalue problem arising from the calculation of the vibration of a membrane is solved using a **ScaLAPACK routine**.

Of course, one would not use these solutions in real applications. Neither is the Jacobi algorithm a state-of-the-art method for the solution of a system of linear equations, nor is the eigensolver from ScaLAPACK the optimal choice for the given problem. Both examples result in a sparse matrix as will be shown in the following. ScaLAPACK contains solvers for full and banded systems, whereas (P)ARACK is a library based on the Arnoldi method which is very suitable for the calculation of a **few** eigenvalues for large **sparse** systems; thus (P)ARPACK would be the natural choice for this kind of problem.

Nevertheless due to the importance of ScaLAPACK for many application fields, e.g. **nanoscience**, and the simplicity of the Jacobi algorithm we present them as illustrative examples.

2 The Poisson Problem

In this section we discuss the numerical solution of the Poisson equation as an example for the approximate treatment of partial differential equations. We give a short outline of

the steps necessary to obtain a serial and later on parallel implementation of the numerical solver. Similar but more elaborate material on this topic can be found in the Refs. 14–16.

In a first step we discuss the discretization of the Poisson equation and introduce one simple solver for the evolving system of linear equations. Afterwards we focus on the parallelization of this algorithm.

2.1 Discretization of the Poisson Equation

The **Poisson equation** in two dimensions is given by

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y) \quad , \quad (x, y) \in \Omega \subset \mathbb{R}^2 \quad (1)$$

where Ω is a domain in \mathbb{R}^2 . For simplicity $u(x, y)$ shall be given on the boundary $\partial\Omega$ by a **Dirichlet boundary condition**

$$u(x, y) = g(x, y) \quad , \quad (x, y) \in \partial\Omega \quad (2)$$

The functions $f(x, y)$ and $g(x, y)$ are given and $u(x, y)$ is to be calculated.

Since the analytic solution of such a partial differential equation might not be feasible depending on the shape of the domain, the functions f, g etc., one often has to resort to the numerical solution of such a differential equation.

In the following we will develop a simple scheme how to calculate u approximately. For this we assume that the domain has a simple form: Ω is a rectangle (Figure 1).

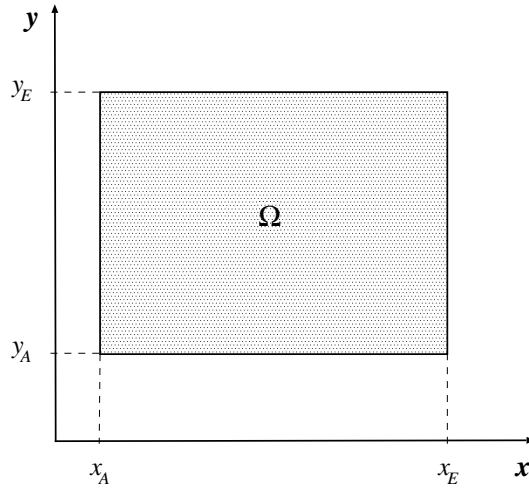


Figure 1. Rectangular domain in \mathbb{R}^2

In order to determine the approximate solution of the Poisson equation, u is calculated at certain points of the rectangle. We impose $\Omega = (x_A, x_E) \times (y_A, y_E)$ with an equidistant mesh (Figure 2), where (x_A, x_E) is divided into $(NI + 1)$ sub-intervals and (y_A, y_E) into $(NJ + 1)$ sub-intervals, $(NI, NJ \in \mathbb{N})$. The mesh width h is then given by

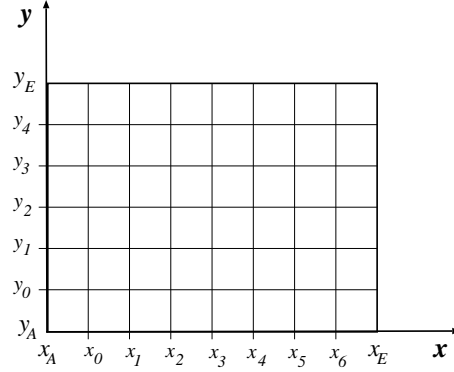


Figure 2. Mesh for $NI = 7$ and $NJ = 5$

$$h = \frac{(x_E - x_A)}{(NI + 1)} = \frac{(y_E - y_A)}{(NJ + 1)} \quad (3)$$

With this choice for the mesh the approximate solution will be calculated at the $NI \cdot NJ$ inner points of the domain (The outer points don't have to be calculated, because they are given by the Dirichlet boundary condition!).

As a next step the second derivatives are replaced by finite differences. For this purpose we use the following Taylor expansions of u at a point (x, y) :

$$u(x + h, y) = u(x, y) + hu_x(x, y) + \frac{h^2}{2!}u_{xx}(x, y) + \frac{h^3}{3!}u_{xxx}(x, y) \pm \dots \quad (4)$$

$$u(x - h, y) = u(x, y) - hu_x(x, y) + \frac{h^2}{2!}u_{xx}(x, y) - \frac{h^3}{3!}u_{xxx}(x, y) \pm \dots \quad (5)$$

Addition of both equations and division by h^2 gives

$$\frac{u(x - h, y) - 2u(x, y) + u(x + h, y)}{h^2} = u_{xx}(x, y) + O(h^2) \quad (6)$$

The result of the analogous procedure for the y -direction is

$$\frac{u(x, y - h) - 2u(x, y) + u(x, y + h)}{h^2} = u_{yy}(x, y) + O(h^2) \quad (7)$$

Using these finite differences the Poisson equation for the $NI \cdot NJ$ inner mesh points of the domain Ω is given by

$$u_{xx}(x_i, y_j) + u_{yy}(x_i, y_j) = f(x_i, y_j) \quad (8)$$

$$(i = 0, \dots, NI - 1 ; j = 0, \dots, NJ - 1)$$

By neglecting the discretization error $O(h^2)$ Eqs. (8) can be written as:

$$u_{i,j-1} + u_{i-1,j} - 4u_{i,j} + u_{i,j+1} + u_{i+1,j} = h^2 f_{i,j} \quad (9)$$

for $i = 0, \dots, NI - 1 ; j = 0, \dots, NJ - 1$. The unknowns

$$u_{i,j} := u(x_i, y_j) \quad (10)$$

have to be calculated from the $NI \cdot NJ$ coupled linear equations (9).

The approximation used here for $u_{xx} + u_{yy}$ is called **5-point stencil** (Figure 3). The name describes the numerical dependency between the points of the mesh. The lexico-

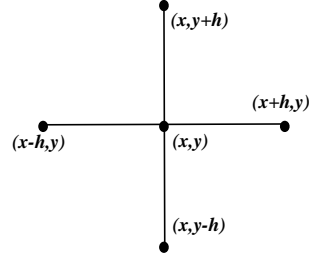


Figure 3. 5-point stencil

graphical numbering (Figure 4) of the mesh points

$$l = j \cdot NI + i + 1 \quad ; i = 0, \dots, NI - 1 \quad ; j = 0, \dots, NJ - 1 \quad (11)$$

and

$$u_l := u_{i,j} \quad (12)$$

allows a compact representation of the system of linear equations by means of a matrix. The coefficient matrix A is a block tridiagonal matrix:

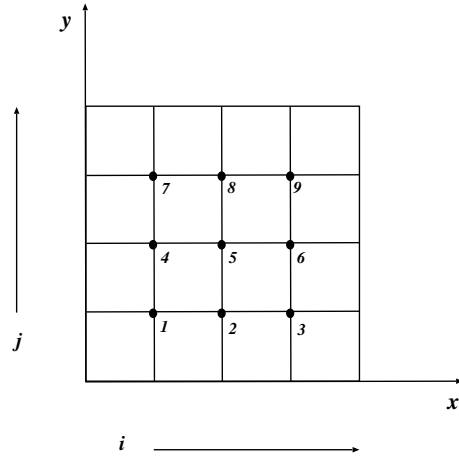


Figure 4. Lexicographical numbering of a 5×5 mesh (with 3×3 inner points)

$$A = \begin{pmatrix} A_1 & I & & & \\ I & A_2 & I & & \\ & \ddots & \ddots & \ddots & \\ & & I & A_{NJ-1} & I \\ & & & I & A_{NJ} \end{pmatrix} \in \mathbb{R}^{(NI \cdot NJ) \times (NI \cdot NJ)} \quad (13)$$

with $A_i, I \in \mathbb{R}^{NI \times NI}$; here I is the unit matrix and

$$A_i = \begin{pmatrix} -4 & 1 & & & \\ 1 & -4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -4 & 1 \\ & & & 1 & -4 \end{pmatrix} \quad i = 1, \dots, NJ \quad (14)$$

This means the task to solve the Poisson equation numerically leads us to the problem to find the solution of a system of linear equations:

$$A \vec{u} = \vec{b} \quad (15)$$

with

$$A \in \mathbb{R}^{(NI \cdot NJ) \times (NI \cdot NJ)} \quad \text{and} \quad \vec{u}, \vec{b} \in \mathbb{R}^{(NI \cdot NJ)} \quad (16)$$

The right hand side \vec{b} contains the $f_{i,j}$ of the differential equations as well as the Dirichlet boundary condition.

For the solution of these coupled linear equations many well-known numerical algorithms are available. We will focus here on the classic but very simple Jacobi algorithm.

2.2 The Jacobi Algorithm for Systems of Linear Equations

Suppose

$$A = D - L - U \quad (17)$$

is a decomposition of the matrix A , where D is the diagonal sub-matrix, $-L$ is the strict lower triangular part and $-U$ the strict upper triangular part. Then for the system of linear equations holds

$$A \vec{u} = \vec{b} \Leftrightarrow (D - L - U) \vec{u} = \vec{b} \Leftrightarrow D \vec{u} = (L + U) \vec{u} + \vec{b} \Leftrightarrow \quad (18)$$

$$\vec{u} = D^{-1}(L + U) \vec{u} + D^{-1} \vec{b} \quad \text{if } D^{-1} \text{ exists.} \quad (19)$$

From Eq. (19) follows the iteration rule (for D non-singular)

$$\vec{u}^{(k)} = D^{-1}(L + U) \vec{u}^{(k-1)} + D^{-1} \vec{b} \quad \text{with } k = 1, 2, \dots \quad (20)$$

This iterative procedure is known as **Jacobi** or **total-step method**. The second name is motivated by the fact that the next iteration is calculated **only** from the values of the unknowns of the last iteration. There are other schemes, e.g. Gauß-Seidel algorithm, which depend on old **and** the current iteration of the unknowns!

The corresponding pseudo code for the serial Jacobi algorithm is given here:

Jacobi algorithm

Choose an initial vector $\vec{u}^{(0)} \in \mathbb{R}^n$

For $k = 1, 2, \dots$

For $i = 1, 2, \dots, n$

$$u_i^{(k)} = \frac{1}{a_{ii}} \left(b_i - \sum_{\substack{j=1 \\ j \neq i}}^n a_{ij} u_j^{(k-1)} \right)$$

The Poisson equation (9) discretized with the **5-point stencil** results in the following iteration procedure

$$\begin{pmatrix} u_1 \\ \vdots \\ \vdots \\ \vdots \\ u_N \end{pmatrix}^{(k)} = -\frac{1}{4} \begin{pmatrix} A'_1 & -I & & & \\ -I & A'_2 & -I & & \\ & \ddots & \ddots & \ddots & \\ & & -I & A'_{NJ-1} & -I \\ & & & -I & A'_{NJ} \end{pmatrix} \begin{pmatrix} u_1 \\ \vdots \\ \vdots \\ \vdots \\ u_N \end{pmatrix}^{(k-1)} - \frac{1}{4} \begin{pmatrix} b_1 \\ \vdots \\ \vdots \\ \vdots \\ b_N \end{pmatrix} \quad (21)$$

with $N = NI \cdot NJ$ and

$$A'_i = \begin{pmatrix} 0 & -1 & & \\ -1 & 0 & -1 & \\ & \ddots & \ddots & \ddots \\ & & -1 & 0 & -1 \\ & & & -1 & 0 \end{pmatrix} \quad i = 1, \dots, NJ \quad (22)$$

This can be seen easily by application of the Jacobi matrix decomposition on the coefficient matrix given by Eqs. (13) and (14). The pseudo code for this special case is shown here

Jacobi algorithm for the Poisson equation

Choose initial vector $\vec{u}^{(0)} \in \mathbb{R}^N$

For $k = 1, 2, \dots$

For $j = 0, 1, \dots, NJ - 1$

For $i = 0, 1, \dots, NI - 1$

$$u_{i,j}^{(k)} = \frac{1}{4} \left(u_{i,j-1}^{(k-1)} + u_{i-1,j}^{(k-1)} + u_{i,j+1}^{(k-1)} + u_{i+1,j}^{(k-1)} - h^2 f_{i,j} \right)$$

2.3 Parallelization of the Jacobi Algorithm

The numerical treatment of the Poisson equation led us to the task to solve a system of linear equations. We introduced the Jacobi algorithm as a simple method to calculate this solution and presented the corresponding serial pseudo code. Now the next step is to discuss strategies **how to implement the Jacobi algorithm on a parallel computer**.

The important point about the Jacobi (total-step) algorithm one has to remember is that the calculation of the new iteration only depends on the values of the unknowns from the **last iteration** as can be seen for instance from Eq. (21). As a consequence the processors of a parallel computer can calculate the new iteration of the unknowns simultaneously, supposed each unknown is assigned to its own processor. This makes the parallelization of the Jacobi algorithm quite easy compared to other methods with more complicated dependencies between different iterations.

Usually the number of unknowns is much larger than the number of available processors. Thus some / many unknowns have to be assigned to one processor, i.e. for our example: the inner points of Ω (Figure 1) are distributed to the available processors. With other words the **domain Ω** is **decomposed** according to a suitable strategy.

The criteria for a “suitable” strategy are

- **load balance**, i.e. same / similar number of unknowns for each processor
- minimization of the **communication** between the processors, i.e. the dependency on unknowns stored on other processors (within one iteration step!) is reduced

For our example, the Poisson equation in two dimensions, a reasonable domain decomposition is shown in Figure 5: Each processor “owns” a domain of the same size, i.e. each

P_{13}	P_{14}	P_{15}	P_{16}
P_9	P_{10}	P_{11}	P_{12}
P_5	P_6	P_7	P_8
P_1	P_2	P_3	P_4

Figure 5. Domain decomposition of a square Ω with 16 processors

P_i “owns” the same number of points. Furthermore the ratio area to edges of each square and consequently the ratio between the number of inner points (no dependency on points “owned” by other processors) to the number of points near the boundary is rather good. This point can be seen even better from Figure 6.

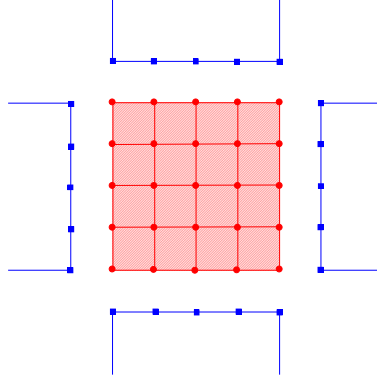


Figure 6. Dependency of the unknowns of processor P_i (red) on values stored on the neighbors (blue)

In Fig. 6 the points / corresponding unknowns of processor P_i are represented by red circles, whereas the blue squares depict the **ghost points**, i.e. points stored on other processors which are required for the calculation of the next iteration of the unknowns on processor P_i .

The dependencies / ghost points shown in Fig. 6 are a result of the 5-point stencil (see Fig. 3) originating from the Laplace operator in Eq. (1). Thus the domain decomposition of choice might differ for other differential equations or other discretization schemes, e.g. finite elements.

Due to the dependencies between the unknowns “owned” by different processors it is clear that the parallelization of the Jacobi algorithm has to introduce statements which will take care of the communication between the processors. One portable way to handle the communication is the widely used **Message Passing Interface (MPI)**¹⁷ library. The pseudo code of the parallel Jacobi algorithm is given here:

Parallel Jacobi algorithm

*Choose initial values for the **own mesh points** and the **ghost points***

Choose initial Precision (e.g. Precision = 10^{10})

While Precision > ε (e.g. $\varepsilon = 10^{-5}$)

1. *Calculate next iteration for the **own domain***
2. *Send the new iteration on **boundary of domain** to **neighboring processors***
3. *Receive the new iteration for the **ghost points***
4. *Calculate Precision = $\|A\vec{u}^{(k)} - \vec{b}\|$*

End While

The steps 2 and 3 show the extension of the serial Jacobi algorithm by *Send* and *Receive* statements. This is of course only one very simple way to implement such a communication with the four neighboring processors. In real applications one will look for more efficient communication patterns.

Step 4 requires implicitly **global communication**, because the vector $\vec{u}^{(k)}$ holding the approximate solution of the system of linear equations is distributed over all processors. As soon as the required precision of the solution is achieved the iteration stops.

3 Vibration of a Membrane

The vibration of a homogeneous membrane is governed by the time-dependent partial differential equation¹⁸

$$\frac{\partial^2 v}{\partial t^2} = \Delta v \quad (23)$$

In order to solve this equation we make a separation ansatz for the time and spatial variables:

$$v(x, y, t) = u(x, y) g(t) \quad (24)$$

By insertion of Eq. (24) into Eq. (23) one immediately obtains

$$g(t) \Delta u(x, y) = u(x, y) g''(t) \Leftrightarrow \quad (25)$$

$$\frac{\Delta u(x, y)}{u(x, y)} = \frac{g''(t)}{g(t)} \quad (26)$$

The left side of Eq. (26) is independent of t , the right side of x, y . Therefore both sides must be equal to a constant $-\lambda$

$$\frac{\Delta u(x, y)}{u(x, y)} = \frac{g''(t)}{g(t)} = -\lambda \Leftrightarrow \quad (27)$$

$$\Delta u(x, y) = -\lambda u(x, y) \quad \text{and} \quad g''(t) = -\lambda g(t) \quad (28)$$

The differential equation for $g(t)$ can be solved easily with the usual ansatz (a linear combination of trigonometric functions).

In the following we want to solve the spatial partial differential equation

$$\Delta u(x, y) = -\lambda u(x, y) \quad (29)$$

numerically. In section 2.1 we presented the discretization of the Poisson equation in two dimensions. In order to allow a re-use of the results derived there, we will calculate the solution of Eq. (29) for a **rectangular** membrane / domain.

Furthermore we choose for simplicity the Dirichlet boundary condition

$$u(x, y) = 0 \quad \text{for } (x, y) \in \partial\Omega \quad (30)$$

Using the same discretization for the Laplace operator and lexicographical numbering of the mesh points / unknowns as in section 2.1 one can see easily that Eq. (29) leads to the **eigenvalue problem**

$$A \vec{u} = -\lambda \vec{u} \quad (31)$$

where the matrix A is given by Eqs. (13) and (14).

In section 2 we presented a simple algorithm for the solution of the system of linear equations and discussed the parallelization by hand. For the eigenvalue problem we choose a different strategy: We make use of a widely used parallel library, namely the **ScaLAPACK** library.

3.1 Parallel Solution Using the ScaLAPACK Library

The largest and most flexible public domain library with linear algebra routines for distributed memory parallel systems up to now is ScaLAPACK¹⁰. Within the ScaLAPACK project many LAPACK routines were ported to distributed memory computers using MPI.

The basic routines of ScaLAPACK are the **PBLAS** (Parallel Basic Linear Algebra Subroutines)¹⁹. They contain parallel versions of the BLAS which are parallelized using **BLACS** (Basic Linear Algebra Communication Subprograms)²⁰ for communication and sequential BLAS for computation. Thus the PBLAS deliver very good performance on most parallel computers.

ScaLAPACK contains direct parallel solvers for dense linear systems (LU and Cholesky decomposition), linear systems with band matrices as well as parallel routines for the solution of linear least squares problems and for singular value decomposition.

Furthermore there are several different routines for the solution of the full symmetric eigenproblem. We will focus in the following on a **simple driver routine** using the QR-algorithm, which computes all eigenvalues and optionally all eigenvectors of the matrix.

Besides this there are other eigensolvers available which are implementations of other algorithms, e.g. a divide-and-conquer routine; an additional expert driver allows to choose a range of eigenvalues and optionally eigenvectors to be computed.

For performance and load balancing reasons ScaLAPACK uses a **two-dimensional block cyclic distribution** for full matrices (see ScaLAPACK Users' Guide)¹³:

First the matrix is divided into blocks of size $MB \times NB$, where MB and NB are the number of rows and columns per block, respectively. These blocks are then uniformly distributed across the $MP \times NP$ **rectangular processor grid** in a cyclic manner. As a result, each process owns a collection of blocks. Figure 7 shows the distribution of a (9×9) matrix subdivided into blocks of size (3×2) distributed across a (2×2) processor grid.

	0		1		0		1		0
0	a_{11}	a_{12}	a_{13}	a_{14}	a_{15}	a_{16}	a_{17}	a_{18}	a_{19}
	a_{21}	a_{22}	a_{23}	a_{24}	a_{25}	a_{26}	a_{27}	a_{28}	a_{29}
	a_{31}	a_{32}	a_{33}	a_{34}	a_{35}	a_{36}	a_{37}	a_{38}	a_{39}
1	a_{41}	a_{42}	a_{43}	a_{44}	a_{45}	a_{46}	a_{47}	a_{48}	a_{49}
	a_{51}	a_{52}	a_{53}	a_{54}	a_{55}	a_{56}	a_{57}	a_{58}	a_{59}
	a_{61}	a_{62}	a_{63}	a_{64}	a_{65}	a_{66}	a_{67}	a_{68}	a_{69}
0	a_{71}	a_{72}	a_{73}	a_{74}	a_{75}	a_{76}	a_{77}	a_{78}	a_{79}
	a_{81}	a_{82}	a_{83}	a_{84}	a_{85}	a_{86}	a_{87}	a_{88}	a_{89}
	a_{91}	a_{92}	a_{93}	a_{94}	a_{95}	a_{96}	a_{97}	a_{98}	a_{99}

Figure 7. Block cyclic 2D distribution of a (9×9) matrix subdivided into (3×2) blocks on a (2×2) processor grid. The numbers outside the matrix indicate processor row and column indices, respectively.

ScaLAPACK as a parallel successor of LAPACK attempts to leave the calling sequence of the subroutines unchanged as much as possible in comparison to the corresponding sequential subroutine from LAPACK. The user should have to change only a few parameters in the calling sequence to use ScaLAPACK routines instead of LAPACK routines.

Therefore ScaLAPACK uses so-called **descriptors**, which are integer arrays containing all necessary information about the **distribution of the matrix**. This descriptor appears in the calling sequence of the parallel routine instead of the leading dimension of the matrix in the sequential one.

For example the sequential simple driver **DSYEV** from LAPACK for the computation of **all eigenvalues** and (optionally) eigenvectors of a **real symmetric** ($N \times N$) matrix **A** has the following calling sequence²¹:

```
...
CALL DSYEV(JOBZ, UPLO, N, A, LDA, W, WORK, LWORK, INFO)
...
```

where **JOBZ** and **UPLO** are characters indicating whether to compute eigenvectors, and whether the lower or the upper triangular part of the matrix **A** is provided. **LDA** is the leading dimension of **A** and **W** is the array of eigenvalues of **A**. The other variables are used as workspace and for error report.

The corresponding ScaLAPACK routine **PDSYEV** is called as follows¹³:

```
...
CALL PDSYEV ( JOBZ, UPLO, N, A, IA, JA, DESCA,
$            W, Z, IZ, JZ, DESCZ, WORK, LWORK, INFO )
...
```

As one can see the leading dimension **LDA** of the LAPACK call is substituted by the indices **IA** and **JA** and the descriptor **DESCA**. **IA** and **JA** indicate the start position of the **global matrix** (usually **IA**, **JA** = 1, but in cases where the global matrix is a sub-matrix of a larger matrix **IA**, **JA** \neq 1 might occur), whereas **DESCA** contains all information regarding the distribution of the global matrix. The parameters **IZ**, **JZ**, and **DESCZ** provide the same information for **Z**, the matrix of the eigenvectors calculated by **PDSYEV**.

In order to use the ScaLAPACK routine the user has to distribute his system matrix in the way required by ScaLAPACK. Thus the user has to setup the **processor grid** by initializing **MP**, the number of processor rows, and **NP**, the number of processor columns. Furthermore one has to choose a suitable blocking of the matrix, i.e. **MB** and **NB**. For many routines, especially for the eigenvalue solvers and the Cholesky decomposition, **MB**=**NB** is mandatory. (Since **MB** and **NB** are crucial for the performance of the solver, one has to use these parameters with care.²²) Further details on the two-dimensional block cyclic distribution of the matrix **A** given by Eqs. (13) and (14) can be found in the appendix.

Once the matrix has been distributed to the processors, the calculation of the eigenvalues and corresponding eigenvectors for the vibration of the rectangular membrane (Eq. (31)) can be calculated easily by one call of the routine **PDSYEV**. Please note that the matrix of the eigenvectors **Z**, is distributed to the processors; thus if necessary, e.g. for output, it is again the task of the user to collect the different local data and to generate the global matrix.

4 Conclusion

In this contribution we presented two examples for the numerical treatment of partial differential equations using parallel algorithms / computers. Both problems were tackled with different strategies: The first example has been solved by means of the simple Jacobi algorithm and a suitable parallelization scheme was discussed. In the second case the parallel calculation has been performed with the help of the ScaLAPACK library.

The pros and cons of the different strategies are obvious. If a suitable parallel library is available and a reorganization of the application software according to the complex data distribution schemes of the libraries is possible, the parallel routines from the library will provide a robust numerical solution with fair or even good performance.

Otherwise the user has to choose a parallelization scheme which best fits his specific application problem and he has to implement the necessary algorithms himself; in order to improve the single processor performance it is still recommendable to use serial library routines, e.g. from BLAS or LAPACK, wherever possible!

Appendix

In section 3.1 some information on the **two-dimensional block cyclic distribution** of the data used by **ScaLAPACK** has been given. In this appendix we will discuss this issue in greater detail.

In Fig. 8 a code fragment is shown which distributes the $N \times N$ matrix given by Eqs. (13) and (14) according to the ScaLAPACK data scheme with block sizes $NB=MB$ to an $MP \times NP$ processor grid. Inclusion of this fragment into a parallel program allows the calculation of the eigenvalues and eigenvectors using the routine **PDSYEV**:

```
...  
      CALL PDSYEV ( JOBZ, UPLO, N, A, IA, JA, DESCA,  
$              W, Z, IZ, JZ, DESCZ, WORK, LWORK, INFO )  
...
```

Notice that in the sequential as well as in the parallel routine the matrix **A** is destroyed. The difference is that in the sequential case if the eigenvectors are requested **A** is overwritten by the eigenvectors whereas in the parallel case the eigenvectors are stored to a separate matrix **Z**.

The matrix **Z** has to be allocated with the same local sizes as **A** and **DESCZ** is filled with the same values as **DESCA**. The size **LWORK** of the local workspace **WORK** can be found in the ScaLAPACK Users' Guide.

The four nested loops in Fig. 8 show how local and global indices can be computed from block sizes, the number of rows and columns in the processor grid and the processor coordinates. The conversion of global to local indices and vice versa is supported by some auxiliary routines in the **TOOLS** sub-library of ScaLAPACK. Here the routine **NUMROC** is used to calculate the number of rows / columns stored on the corresponding processor.

There is also a sub-library **REDIST** of ScaLAPACK which allows the redistribution of any two-dimensional block cyclically distributed matrix to any other block cyclic two-dimensional distribution. Thus if **A** was column cyclically distributed or if the eigenvectors have to be column cyclically distributed for further computations they can be redistributed

```

! Create the MP * NP processor grid
CALL BLACS_GRIDINIT( ICTXT, 'Row-major', MP, NP)
! Find my processor coordinates MYROW and MYCOL
! NPROW returns the same value as MP,
! NPCOL returns the same value as NP
CALL BLACS_GRIDINFO( ICTXT, NPROW, NPCOL, MYROW, MYCOL)
! Compute local dimensions with routine NUMROC from TOOLS
! N is dimension of the matrix
! NB is block size
MYNUMROWS = NUMROC( N, NB, MYROW, 0, NPROW )
MYNUMCOLS = NUMROC( N, NB, MYCOL, 0, NPCOL )
! Local leading dimension of A,
! Number of local rows of A
MXLLDA = MYNUMROWS
! Allocate only the local part of A
ALLOCATE( A( MXLLDA, MYNUMCOLS ) )
! Fill the descriptors, P0 and Q0 are processor coordinates
! of the processor holding global element A(1,1)
CALL DESCINIT( DESCA, N, N, NB, NB, P0, Q0, ICTXT, MXLLDA, INFO )
! Fill the local part of the matrix with data
do j = 1, MYNUMCOLS, NB ! Fill the local column blocks
  do jj = 1, min( NB, MYNUMCOLS - j + 1 ) ! all columns of one block
    jloc = j - 1 + jj ! local column index
    jglob = (j - 1) * NPCOL + MYCOL * NB + jj ! global column index
    do i = 1, MYNUMROWS, NB ! local row blocks in column
      do ii = 1, min( NB, MYNUMROWS - i + 1 ) ! rows in row block
        iloc = i - 1 + ii ! local row index
        iglob = (i - 1) * NPROW + MYROW * NB + ii ! global row index
        A( iloc, jloc ) = 0
        If ( iglob == jglob ) A( iloc, jloc ) = -4
        If ( iglob == jglob + 1 .and. mod( jglob, NI ) /= 0 ) &
                                     A( iloc, jloc ) = 1
        If ( jglob == iglob + 1 .and. mod( iglob, NI ) /= 0 ) &
                                     A( iloc, jloc ) = 1
        If ( iglob == jglob + NI ) A( iloc, jloc ) = 1
        If ( jglob == iglob + NI ) A( iloc, jloc ) = 1
      enddo
    enddo
  enddo
enddo

```

Figure 8. Code fragment which distributes the matrix given by Eqs. (13) and (14) according to ScaLAPACK (It is assumed that $MB=NB=NI$ and $N=NI \cdot NJ$).

by such a routine, as a column cyclic distribution is nothing else but a block cyclic two-dimensional distribution to a $1 \times \text{NPR}$ (with NPR = number of processors) grid with block size 1.

References

1. J. J. Dongarra, I. S. Duff, D. C. Sorensen, and H. A. van der Vorst, *Numerical Linear Algebra for High-Performance Computers*, SIAM, Philadelphia (1998).
2. <http://gams.nist.gov/Classes.html> and especially <http://gams.nist.gov/serve.cgi/Class/D/>
3. B. Wilkinson and M. Allen, *Parallel Programming: Techniques and Applications using networked Workstations and Parallel Computers*, Pearson, Upper Saddle River (2005).
4. A. Grama, A. Gupta, G. Karypis, and V. Kumar, *Introduction to Parallel Computing*, Pearson, Harlow (2003).
5. M. Bücker, *Iteratively Solving Large Sparse Linear Systems on Parallel Computers in Quantum Simulation of Complex Many-Body Systems: From Theory to Algorithms*, J. Grotendorst et al. (Ed.), John von Neumann Institute for Computing, NIC Series Vol. **10**, 521-548 (2002)
<http://www.fz-juelich.de/nic-series/volume10/buecker.pdf>
6. B. Lang, *Direct Solvers for Symmetric Eigenvalue Problems in Modern Methods and Algorithms of Quantum Chemistry*, J. Grotendorst (Ed.), John von Neumann Institute for Computing, NIC Series Vol. **3**, 231-259 (2000).
<http://www.fz-juelich.de/nic-series/Volume3/lang.pdf>
7. B. Steffen, *Subspace Methods for Sparse Eigenvalue Problems in Modern Methods and Algorithms of Quantum Chemistry*, J. Grotendorst (Ed.), John von Neumann Institute for Computing, NIC Series Vol. **3**, 307-314 (2000).
<http://www.fz-juelich.de/nic-series/Volume3/steffen.pdf>
8. <http://www.netlib.org/blas/>
9. <http://www.netlib.org/lapack/>
10. <http://www.netlib.org/scalapack/>
11. <http://www.caam.rice.edu/software/ARPACK/>
12. <http://www-unix.mcs.anl.gov/petsc/petsc-as/>
13. L. S. Blackford, J. Choi, A. Cleary et al., *ScaLAPACK Users' Guide*, SIAM, Philadelphia (1997).
14. G. Ahlefeld, I. Lenhardt, and H. Obermaier, *Parallele numerische Algorithmen*, Springer, Berlin (2002).
15. J. M. Ortega, *Introduction to parallel and vector solution of linear systems*, Plenum Press, New York (1988).
16. J. Zhu, *Solving partial differential equations on parallel computers*, World Scientific, Singapore (1994).
17. W. Gropp, E. Lusk, and A. Skjellum, *Using MPI : Portable Parallel Programming with the Message-Passing Interface*, MIT Press, Cambridge (1994).
18. R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Volume I, Interscience Publishers, New York (1953).
19. http://www.netlib.org/scalapack/pblas_gref.html

20. J. J. Dongarra and R. C. Whaley, *A User's Guide to the BLACS*, LAPACK Working Note **94** (1997).
<http://www.netlib.org/lapack/lawns/lawn94.ps>
21. E. Anderson, Z. Bai, C. Bischof et al., *LAPACK Users' Guide, Second Edition*, SIAM, Philadelphia (1995).
22. I. Gutheil, *Basic Numerical Libraries for Parallel Systems* in Modern Methods and Algorithms of Quantum Chemistry, J. Grotendorst (Ed.), John von Neumann Institute for Computing, NIC Series Vol. **3**, 47-65 (2000).
<http://www.fz-juelich.de/nic-series/Volume3/gutheil.pdf>